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On the Convergence of the Jacobi-Davidson Method – Based on a Shift Invariance Property

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Abstract

Jacobi-Davidson type methods have been recently proposed for the iterative compution of a few eigenpairs of a large-scale and sparse matrix. This type methods are characterized by the correction equation for generating a subspace where eigenpairs are approximated. In this report, we present a shift invariance property of the Krylov subspace on a projected space. Based on the property, a procedure for solving the correction equation is proposed. Through the procedure, we can construct not only existing methods but also new methods of Jacobi-Davidson type.

1 Introduction

Given an $N \times N$ large and sparse matrix A, we consider computing a few eigenpairs ($\lambda \in \mathbb{C}, \boldsymbol{x} \in \mathbb{C}^N$) satisfying

$$A\boldsymbol{x} = \lambda \boldsymbol{x} \quad (\boldsymbol{x} \neq \boldsymbol{0}). \tag{1}$$

For the iterative computation of eigenpairs, Krylov subspace methods are widely used, e.g., the Lanczos method [7, 2] (when A is Hermitian) and the Arnoldi method [1, 2] (when A is non-Hermitian). On the other hand, a different type of iterative methods have been recently proposed, e.g., the Jacobi-Davidson (JD) method [10, 5, 2] and the Riccati method [3]. This type methods are characterized by the correction equation [10] for generating a subspace. Here, we focus on this type methods and call them JD-type methods.

In JD-type methods, the correction equation is (approximately) solved for generating a basis vector of a subspace. According to solvers for the equation, different subspaces are generated, i.e., different JD-type methods are produced. In this report, we present a shift invariance property of the Krylov subspace on a projected space [8]. Based on the property, a procedure for solving the correction equation is proposed. Through the procedure, not only existing JD-type methods but also new JD-type methods can be constructed. Relationship among the constructed methods are established.

This report is organized as follows. In section 2, we describe the correction equation in JD-type methods. In section 3, we present our procedure for solving the correction equation. Through the procedure, JD-type methods can be constructed. In section 4, numerical experiments are reported to compare JD-type methods. Finally, we summarize this report in section 5. Throughout this report, I denotes the $N \times N$ identity matrix, and $(\cdot)^*$ denotes the conjugate transpose. Let $\mathcal{K}_m(A, \boldsymbol{b})$ denote the m-dimensional Krylov subspace span$\{\boldsymbol{b}, A\boldsymbol{b}, \ldots, A^{n-1}\boldsymbol{b}\}$.

2 JD-type methods

To start with, we describe the correction equation in JD-type methods. The equation is a reformulation of Jacobi's idea [6] for generating a subspace. Then, the JD method and the Riccati method are outlined.

2.1 The correction equation

Let Q be an $N \times k$ matrix whose column vectors form an orthonormal basis of a subspace $\mathcal{Q}$. Let $(\theta, \boldsymbol{u})$ be an approximate eigenpair. We consider $\boldsymbol{u} \in \mathcal{Q}$, i.e., $\boldsymbol{u} = Q\boldsymbol{y}$ $(\boldsymbol{y} \in \mathbb{C}^k)$. The Rayleigh quotient of $\boldsymbol{u}$ is taken as the approximate eigenvalue $\theta = \boldsymbol{u}^* A \boldsymbol{u}$ with $\|\boldsymbol{u}\|_2 = 1$. We define the residual vector $\boldsymbol{r} = A\boldsymbol{u} - \theta\boldsymbol{u}$ and compute $\|\boldsymbol{r}\|_2$ to check the accuracy of $(\theta, \boldsymbol{u})$.

Here, we are given the approximate eigenpair $(\theta, \boldsymbol{u})$ to $(\lambda, \boldsymbol{x})$. To get the exact eigenvector $\boldsymbol{x}$, Jacobi's idea is to find the correction vector $\boldsymbol{t} = \boldsymbol{x} - \boldsymbol{u}$ satisfying $\boldsymbol{t} \perp \boldsymbol{u}$. From Eq. (1), $\boldsymbol{t}$ satisfies

$$A(\boldsymbol{u} + \boldsymbol{t}) = \lambda(\boldsymbol{u} + \boldsymbol{t}). \tag{2}$$

Let $P = I - \boldsymbol{u}\boldsymbol{u}^*$, then applying the projector P to Eq. (2) leads to the correction equation [10] as follows

$$P(A - \lambda I)P\boldsymbol{t} = -\boldsymbol{r}. \tag{3}$$

The unknown eigenvalue λ exists in Eq. (3). To vanish λ, the projector $I - P$ is applied to Eq. (2). This leads to

$$\lambda = \boldsymbol{u}^* A \boldsymbol{u} + \boldsymbol{u}^* A \boldsymbol{t}. \tag{4}$$

From Eqs. (3) and (4), a Riccati form [3] of the correction equation is derived as follows

$$P(A - (\theta + \boldsymbol{u}^* A\boldsymbol{t})I)P\boldsymbol{t} = -\boldsymbol{r}. \tag{5}$$

In JD-type methods, the correction vector $\boldsymbol{t}$ is approximated and the approximation is used to expand the subspace $\boldsymbol{Q}$. In the expanded subspace, the eigenpair will be approximated again.

2.2 Solving the correction equation

Two JD-type methods are briefly described here. One is the Riccati method, the other is the JD method.

The Riccati method approximates the solution vector of nonlinear equation (5) in a Krylov subspace [3]. On the other hand, typically in the JD method, Eq. (5) is linearized and the following linear system

$$P(A - \theta I)P\boldsymbol{t} = -\boldsymbol{r} \tag{6}$$

is approximately solved by the GMRES algorithm [9]. The JD method discards the term $\boldsymbol{u}^* A\, \boldsymbol{t}$. From this difference, the Riccati method may show faster convergence than the JD method.

3 Constructing JD-type methods

Our approach for computing the correction vector is outlined as follows.

- Replace the unknown eigenvalue λ in Eq. (3) by its approximation σ.
- Solve the following linear system

$$P(A - \sigma I)P\boldsymbol{t} = -\boldsymbol{r}. \tag{7}$$

To this end, double Krylov subspaces are used as follows.

- The first subspace $\mathcal{K}_m(A, \boldsymbol{u})$ for σ.
- The second subspace $\mathcal{K}_n(P(A-\sigma I)P, \boldsymbol{r})$ for solving Eq. (7) approximately.

3.1 Shift invariance property

The computational cost of the approach is considerable, especially in matrix-vector multiplications for generating the basis vectors of the double Krylov subspaces. To save these costs, we make clear a relationship of the subspaces.

It is known that the Krylov subspace is shift invariant, i.e.,

$$\mathcal{K}_n(A - \sigma I, \boldsymbol{b}) = \mathcal{K}_n(A, \boldsymbol{b}).$$

We show that the property holds on a projected space [8].

Theorem 1 *Let G be an $N \times N$ matrix satisfying $G^2 = G$, $G^* = G$. Then, the Krylov subspace on a projected space is shift invariant, that is*

$$\mathcal{K}_n(G^*(A - \sigma I)G, G\boldsymbol{b}) = \mathcal{K}_n(G^*AG, G\boldsymbol{b}). \tag{8}$$

Corollary 1 *From Eq.* (8), *the double Krylov subspaces satisfy*

$$\mathcal{K}_n(P(A - \sigma I)P, \boldsymbol{r}) = P\mathcal{K}_{n+1}(A, \boldsymbol{u}). \tag{9}$$

From Eq. (9), the basis of the first subspace can be reused as that of the second subspace. The computational cost for generating the basis are therefore saved.

3.2 Procedure for the correction equation

By utilizing the relationship of the double Krylov subspaces, our approach is outlined as follows.

Krylov procedure for the correction equation (7)

Step 1. Set parameters m, n, and $\ell = \max(m, n+1)$.

Step 2. Generate ℓ-orthonormal basis vectors $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_\ell$ of $\mathcal{K}_\ell(A, \boldsymbol{u})$.

Step 3. Set the algorithm to generate the approximate eigenvalue σ in
$\mathcal{K}_m(A, \boldsymbol{u}) = \mathrm{span}\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_m\}$.

Step 4. Set the algorithm to solve Eq. (7) approximately in
$\mathcal{K}_n(P(A - \sigma I)P, \boldsymbol{r}) = \mathrm{span}\{\boldsymbol{v}_2, \ldots, \boldsymbol{v}_{n+1}\}$.

Through the procedure, JD-type methods can be constructed by the decision of the parameters, i.e., m, n and the two algorithms at Steps 3 and 4. Examples of the constructed methods are shown in Table 1.

Table 1: The parameter decision for JD-type methods.

Type	m	Algorithm at Step 3	Algorithm at Step 4
(I)	1	Rayleigh quotient	n-steps of Shifted GMRES
(II)	$n+1$	Arnoldi (Ritz)	n-steps of Shifted FOM
(III)	$n+1$	Arnoldi (Ritz)	n-steps of Shifted GMRES
(IV)	$n+1$	Arnoldi (Harmonic)	n-steps of Shifted GMRES

The existing JD-type methods are reconstructed through the procedure.

Remark 1 *Suppose the JD method is set up with the n-steps of the GMRES algorithm for solving Eq.* (6) *approximately. Then, the JD method is equivalent to the JD-type (I) method in Table 1.*

Remark 2 *Suppose the Riccati method is set up with the n-dimensional Krylov subspace for solving Eq.* (5) *approximately. Then, the Riccati method is equivalent to the JD-type (II) method in Table 1.*

From the above remarks, we compare the JD method with the Riccati method. At Step 2 in the Krylov procedure, $\ell = n + 1$ dimensional subspace is generated in the both methods. At Step 3, the JD method utilizes only $m = 1$ dimensional subspace whereas the Riccati method utilizes the maximum $m = n+1$ dimensional subspace. Hence, in the Riccati method, a better approximate eigenvalue σ can be set in Eq. (7). As a result, a better approximation of the correction vector may be produced in the Riccati method. For this reason, the Riccati method may show faster convergence than the JD method. However, in the Riccati method, the Arnoldi algorithm producing Ritz values is implicitly used at Step 3. This may not be appropriate when desired eigenvalues are interior.

We consider constructing other JD-type methods, e.g., Type (III) and (IV) in Table 1. The parameter m is the same as that in the Riccati method to utilize the maximum dimensional subspace at Step 3 for approximate eigenvalues. In the Arnoldi algorithm at Step 3, Ritz values are produced for exterior eigenvalues (Type (III)) whereas harmonic Ritz values are produced for interior eigenvalues (Type (IV)). To produce the minimum residual solution of Eq. (7), the shifted GMRES algorithm is adopted at Step 4 (Type (III) and (IV)).

4 Numerical experiments

We show numerical experiments to compare the three kinds of JD-type methods. The JD method approximately solved Eq. (6) by the $n = 10$ steps of the GMRES algorithm. The Riccati method approximately solved Eq. (5) in the $n = 10$ dimensional Krylov subspace. The JD-type (III) method approximately solved Eq. (7) with the parameter $n = 10$. Number of matrix-vector multiplications per iteration were the same in all the methods.

By using these methods, we computed the largest eigenvalue and its corresponding eigenvector of the real nonsymmetric matrix DW8192 obtained from [4]. These experiments were implemented with Fortran 77 in double precision arithmetic on AMD Phenom 9500 (2.2 GHz). In the three methods, an initial approximate eigenvector was given by a common vector whose elements were random numbers. Iteration was stopped when the relative residual 2-norm $\| \boldsymbol{r} \|_2 / |\theta| \le 10^{-12}$. Convergence histories are shown in Figure 1.

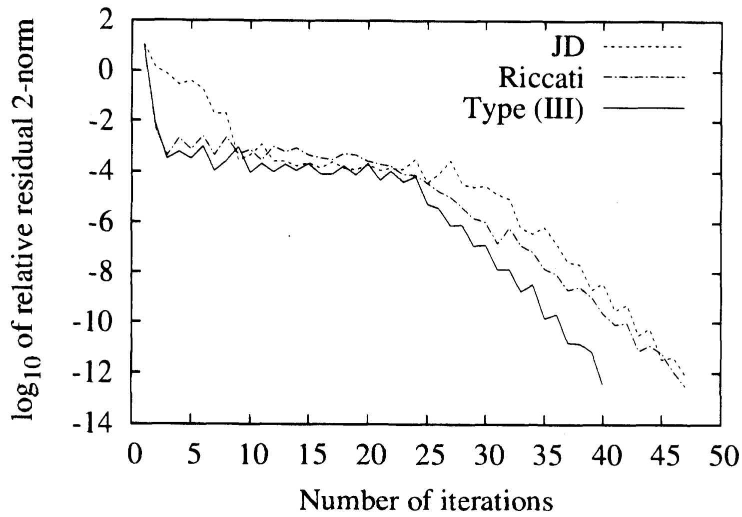

Figure 1: Convergence histories of relative residual 2-norms.

As shown in Figure 1, the Type (III) method showed faster convergence than both the JD method and the Riccati method. With respect to computational time, the JD method required 2.17 seconds, the Riccati method required 2.25 seconds, and the Type (III) method required 1.60 seconds.

5 Conclusion

In this report, we present a shift invariance property of the Krylov subspace on a projected space. By utilizing the property, we provide a procedure for solving the correction equation. Through the procedure, not only existing JD-type methods but also new JD-type methods can be constructed. Numerical experiments indicates that the new JD-type method is a good competitor to existing JD-type methods.

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